## Close out and Final report for NASA Glenn Cooperative Agreement NCC3-965

## Computational Material Processing in Microgravity

### DPIMS Space Experiment

Working with Professor David Matthiesen at Case Western Reserve University (CWRU) a computer model of the DPIMS (Diffusion Processes in Molten Semiconductors) space experiment was developed that is able to predict the thermal field, flow field and concentration profile within a molten germanium capillary under both ground-based and microgravity conditions as illustrated in Figure 1. These models are coupled with a novel nonlinear statistical methodology for estimating the diffusion coefficient from measured concentration values after a given time that yields a more accurate estimate than traditional methods. This code was integrated into a web-based application that has become a standard tool used by engineers in the Materials Science Department at CWRU.

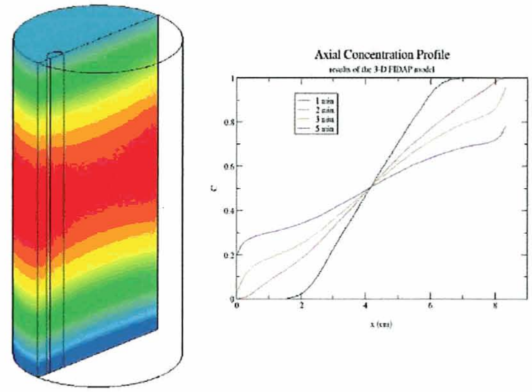


**Figure 1. 3D Model of DPIMS space experiment.**

### Ripple Turbulence

A custom three-dimensional spectral code was developed to predict the dynamics of a rather large (10 cm diameter) water drop freely suspended in space and subjected to acoustic or air-jet forcing. This was done in collaboration with Seth Putterman of UCLA, the principal investigator of the ripple turbulence space experiment, in order to improve the design of that experiment. A finite element model of this process had already been developed previously using the commercial code FIDAP, but this model was restricted to axisymmetric oscillations and did not scale well into the fully three dimensional cases. The free surface shape predicted by the FIDAP model for a typical forcing case is shown in Figure 2 for three successive times. At a certain level of forcing, it is more likely that energy would flow into the fully three-dimensional surface modes. In fact, this is a requirement for the onset of ripple turbulence. The custom three-dimensional spectral model is able to account for this but it would require further optimization before it can be successfully used to predict the droplet shape at the onset of ripple turbulence. Even so, it is a very useful tool for studying the lower-order dynamics of fully three dimensional droplets in space.

**Figure 2. Forced oscillations of a large water drop in microgravity.**

### Fluctuating Hydrodynamics

A thermal strain model was developed of the fluctuating hydrodynamics space experiment of David Cannell at UCSB. The parameters of this model were varied in order to find the optimal

experimental design with the most uniform temperature distribution and minimal thermal strain. This was an important requirement because their optical detection method could be compromised by any thermal "lensing" effects. This model showed that the upper and lower surfaces of the mirror are warped into a spherical shape having the same radius of curvature, and the deflections were on the order of 0.5 Angstroms, much smaller than the wavelength of light used in the optical detector (Figure 3). Additional models were used to optimize the final design and to suggest numerous improvement. In this way, potential problems were avoided before any costly fabrication.

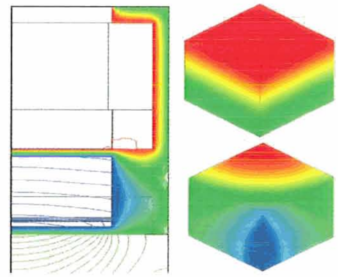

**Figure 3. 3D thermal strain model.**

## Protein Crystal Growth in a Microchannel

A model of protein crystallization in a microchannel was developed in collaboration with Dr. Larry DeLucas, Director of the Center for Biophysical Sciences and Engineering at the University of Alabama at Birmingham. The particular device under consideration is the TOPAZ Protein Crystal Growth Chip by Fluidigm. In this device two microwells are connected by a microchannel (100 microns wide, 500 microns long) as shown in Figure 4. One microwell is filled with a protein rich solution while the other well is filled with a salt-rich solution. The two solutions are allowed to mix over time, and the final equilibrium concentrations are controlled by changing the relative volumes of the microwells. The supersaturation level is dictated by the local salt and protein concentrations, and protein crystals will start to form in the channel and wells. This process works fairly well except that, as it is, the rate of crystallization is too fast, and a slower growth rate is desired because it yields larger, higher-quality crystals. This model is being used to explore different design changes and/or process changes that will lead to higher quality crystals. Methods that were explored included opening and closing the barrier between the two wells periodically.

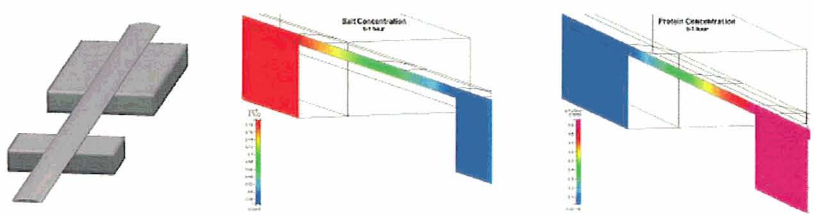


**Figure 4. Model of the TOPAZ Protein Crystal Growth Chip by Fluidigm.**

## Drug Permeability

One of the important characteristic properties of any pharmaceutical drug is its permeability, the rate at which it crosses a porous membrane such as the gastrointestinal tract and the blood-brain barrier. One commonly-used method for estimating the in-vivo permeability is known as PAMPA, parallel artificial membrane permeability assay. Using this approach, the permeability across an artificial membrane is estimated by measuring the average amount of drug that crosses the membrane after a prescribed period of time. Despite its popularity, this approach is based on an oversimplified model that assumes a uniform concentration on both sides of the membrane except for within a thin boundary layer right next to the membrane referred to as the Unstirred Water Layer (UWL). Dr. Panzarella has developed several improved models (both analytical as

well as computational) of this process by rigorously accounting for all of the transport mechanisms involved (Figure 5). Using these improved models, better estimates of the permeability can be obtained.

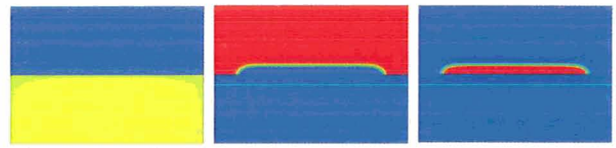

**Figure 5. Analysis of the PAMPA permeability experiment.**

## Rapid Design and Simulation Tools for Space-Bound Biochip Devices

### *Microfluidic Water Quality Sensor (JPL)*

Numerical models are aiding in the design of a microfluidic water quality sensor being developed by the Space Microsensors Group at the Jet Propulsion Laboratory. This sensor will measure the concentration of dissolved ions by first separating them based on their different electric mobilities and then measuring the electrical conductivity and relating that to the ion concentration. The initial design consisted of a long microchannel covering an interdigitated array of electrodes. By alternately charging and discharging the electrodes, ions move towards and away from the electrodes at different speeds depending on their relative electrical mobilities. By applying a forward flow along the microchannel, the ions experience different average drift speeds and separation is slowly and gradually achieved over many cycles.

There are a number of issues that have arisen during the design process that have prompted the development of several numerical models to help resolve those issues. The principal objective is to find the optimal set of parameter values that will maximize ion separation. These parameters include the height, width and length of the separation channel, the placement and dimensions of the electrodes, the applied voltage and the operation frequency. Alternate electrode configurations are being considered as well. In fact, based upon preliminary modeling results, the interdigitated electrode configuration was replaced by a simpler configuration consisting of just two electrodes placed across from each other on opposite sides of the microchannel. This configuration is easier to analyze and has more desirable properties. Numerical models have also determined the electrode shielding time for this configuration, which is useful since the optimal operation frequency is essentially the inverse of the shielding time. Something else of interest to the designers is the critical voltage necessary to completely remove ions from the bulk solution, and this is also something the numerical models are capable of readily determining. A dimensional analysis was also used to help guide the design in a more rational way by reducing the number of independent parameters.

### *Bubble Management in Microgravity*

The presence of suspended gas bubbles in microgravity fluids is a persistent problem that has plagued numerous space experiments in the past and poses a serious obstacle to future environmental monitoring devices. These devices are being built upon microfluidic technology because of the need for smaller, lighter and more efficient devices. Bubbles in microfluidic devices are a particular problem since the bubble diameter is often on the order of the channel dimensions, and this will seriously affect the detection process. Thus, some means for separating the gas bubbles from the sample liquids is required. Unfortunately, no comprehensive strategy for bubble management has yet been identified and verified. Because of this, an effort was made

to focus on the development of a number of practical bubble management strategies that can be applied as a sample preparation stage to any microfluidic device intended for space application.

So far, a number of conceptual bubble management strategies have been developed and preliminary testing with numerical simulations has shown them to be quite plausible. The key element of these designs is the ability to achieve separation with a minimum application of force over short distances and over short periods of time. These strategies fall into two general categories: (1) prevention of bubbles from entering the device during initial sample collection, and (2) active separation of bubbles that are already within the microfluidic system. Three separation principles are being considered based on thermocapillary, dielectrophoretic and mechanical forces.

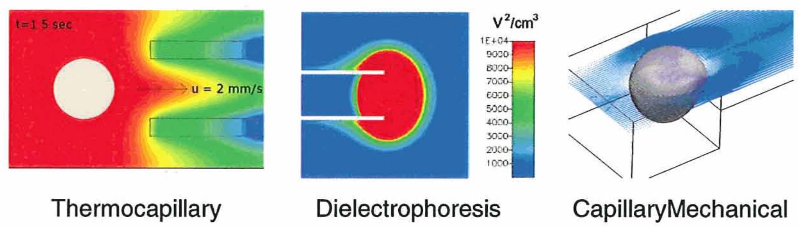


**Figure 6. Simulations of Air Bubble Management in Microfluidic Devices.**

For example, it has been shown that by cooling a needle with respect to the surrounding liquid, bubbles are pushed back from the needle tip due to thermocapillary forces while liquid is being drawn in. Numerical simulations have shown this method to work quite well in surfactant-free systems. An alternate method is based on dielectrophoresis. A dielectric needle is coated on the inner and outer surfaces with a thin metallic film, and by applying a voltage between the inner and outer electrodes, a strong electric field is produced near the tip which repels the gas bubbles (due to negative dielectrophoretic forces) during liquid withdrawal. Numerous other strategies are also being considered based on these same separation principles but with different configurations. Numerical simulations have already demonstrated the plausibility of some of these approaches, and further numerical simulations will be used to test others.

### *Optimization of DNA Hybridization in a Microchannel*

A model of DNA surface hybridization, which forms the basis of many biosensors (Figure 7), was developed in collaboration with the relatively young biotech company HealthSpex. The model is of a particular process consisting of circular patches of oligonucleotides deposited and immobilized onto the surface of a glass slide over which microchannels are affixed carrying sample fluid. If the DNA strands in the sample fluid hybridize (bind) with the immobilized DNA, this can be detected optically. One of the biggest problems with this method is being able to identify strands that may be close, but not exact, matches. One way of doing this is to exploit the changes in the thermodynamics of the binding process with respect to temperature. Thus, by imposing a temperature gradient across the slide, different optical patterns can be created and hopefully used to distinguish between perfect and near-perfect matches. A software package was developed that automatically computes the thermodynamic properties of an oligonucleotide from empirical data, and this was incorporated into

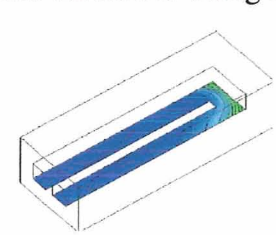

**Figure 7. Model of DNA Hybridization in a Microchannel.**

computational models of the transport mechanisms in the microchannel in order to optimize this process.

### *Development of Electronic Biosensors*

Work was also done in both the theoretical and experimental aspects of a new research program recently started here at NASA Glenn for electronic biosensor design. These biosensors will be able to detect trace levels of biological contamination in food and water supplies, something that is absolutely vital for the safety of the astronauts during long-duration space missions. Work has been done with the lead scientist of BSD, a small start-up company with an innovative biosensor design, to develop this sensor and adapt it for NASA's use. A working prototype has been developed capable of detecting e. coli bacteria in sample fluids, but it still needs much optimization before it can be used in the field. The response of this biosensor to multiple injections of e. coli is shown in Figure 8. The presence of the bacteria is indicated by the voltage spikes due to an interaction with a specially-coated aluminum sensor strip. This type of electronic sensor is a considerable breakthrough in this field due to its simplicity and nearly-immediate response time. The best alternative sensors available at present take a minimum of 8 hours to obtain a result.

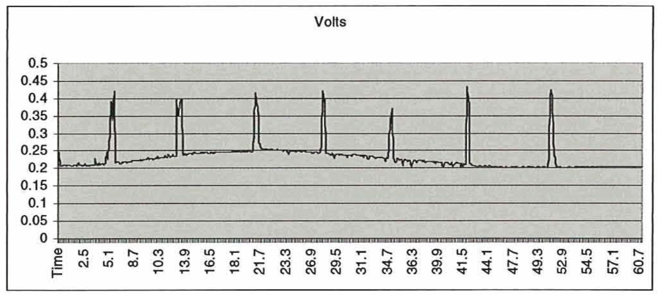


**Figure 8. Voltage spikes corresponding to injections of**

## Optimization of Airborne VHP Decontamination

A collaboration was established with STERIS, Inc. to optimize their patented VHP (Vaporous Hydrogen Peroxide) building decontamination technology with the help of custom computer models developed under this grant. STERIS is perhaps most well known for using this technology to decontaminate the US postal facilities in DC and Virginia that were infected with Anthrax. Despite their eventual success, it took over two years to complete because of numerous process inefficiencies. The key element of this process is the need to distribute VHP to every corner and crevice of the room with a high enough concentration and for a long enough period of time to completely eradicate the contaminant. The chemistry of this process is already well understood, but the transport mechanisms are not.

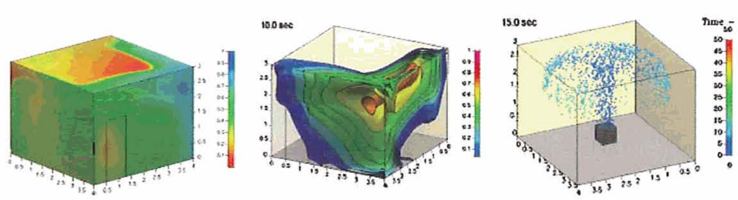

**Figure 9. Model of building decontamination for Steris.**

To optimize the transport process, computer models were developed to simulate the dispersal of VHP within closed environments. A modular programming platform was developed for rapidly building models by assembling common objects such as tables, chairs, cabinets, etc. into a room

enclosure with a minimum of effort. A typical room built in this manner is shown in Figure 10 along with the results of a decontamination simulation in that room. The red areas on the wall are the "trouble spots" where contamination still remains. This model is being used to determine the optimal placement of the vaporizer unit and any auxiliary fans ahead of time to ensure complete decontamination. This saves time and money by reducing the number of trial-and-error cycles normally required. Also shown in Figure 10 is a simulation of the air flow produced by a vaporizer and two fans for a particular room (Room 113) in an actual nearby Army test facility. The colored lines indicate the path taken by the VHP molecules as they leave the vaporizer and pass through the fans. This model was used to determine the optimal number and placement of the fans to maximize wall coverage. The results of this model compare favorably with experimental measurements.

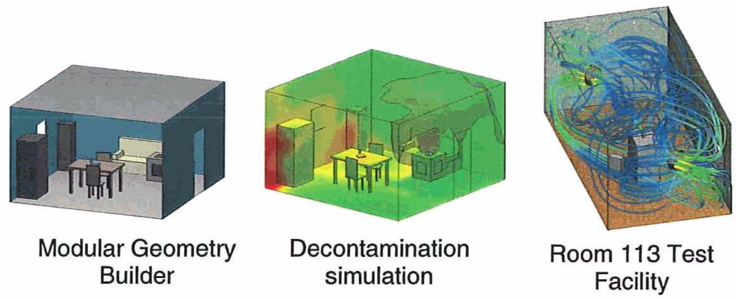


**Figure 10. Model of building decontamination for STERIS.**

22800 Cedar Point Road • Cleveland, Ohio 44142 • p: 440.962.3000 • f: 440.962.3120 • www.oai.org

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Attached you will find the Final Report for the Cooperative Agreement NCC3-965. This will complete the close-out requirements accordingly to NASA policy.

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| Researcher(s): | Charles H. Panzarella |
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If there are any questions concerning this Final Report, please contact the Ohio Aerospace Institute Accounting Manager, Sue Horst at 440.962.3041.

Ann O. Heyward
Ohio Aerospace Institute
Vice President, Workforce Enhancement

Distribution:

Andrew H. Cole
Contract Administrator
Office of Naval Research
Chicago Regional Office
230 S. Dearborn Ave., Room 380
Chicago, IL 60604-1595

Center for Aerospace Information
Attn: Document Processing Section
7121 Standard Drive
Hanover, MD 21076

Ms. Saundra Gage
Grant Administrator
NASA Glenn Research Center
21000 Brookpark Road
Mail Stop 500-319
Cleveland, OH 44135

Arnon Chait
Technical Officer
NASA Glenn Research Center
21000 Brookpark Road
Mail Stop 105-1
Cleveland, OH 44135

Ohio Aerospace Institute
22800 Cedar Point Road
Cleveland, OH 44142

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